=> FILE REG
FILE 'REGISTRY' ENTERED AT 14:59:12 ON 14 AUG 2003

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 13 AUG 2003 HIGHEST RN 566135-25-9
DICTIONARY FILE UPDATES: 13 AUG 2003 HIGHEST RN 566135-25-9

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2003

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

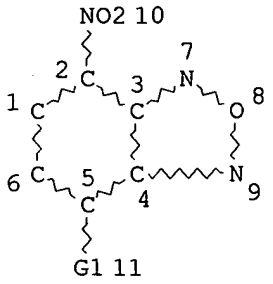
Experimental and calculated property data are now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details:
http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf

=> FILE HCAPLU
FILE 'HCAPLUS' ENTERED AT 14:59:16 ON 14 AUG 2003

FILE COVERS 1907 - 14 Aug 2003 VOL 139 ISS 7
FILE LAST UPDATED: 13 Aug 2003 (20030813/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> D QUE
L25 STR



1688 structures from query

VAR G1=O/S/N
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 11

STEREO ATTRIBUTES: NONE
L27 1688 SEA FILE=REGISTRY SSS FUL L25
L28 1108 SEA FILE=HCAPLUS ABB=ON L27
L32 9 SEA FILE=HCAPLUS ABB=ON L28 AND (SILK OR WOOL OR FUR OR HAIR OR KERAT?)

9 CA references with utility

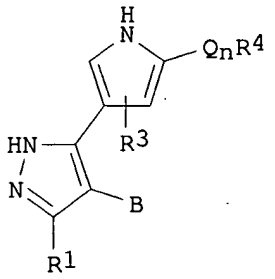
=> D L32 ALL 1-9 HITSTR

L32 ANSWER 1 OF 9 HCAPLUS COPYRIGHT 2003 ACS on STN
AN 2003:117818 HCAPLUS
DN 138:153530
TI Preparation of pyrazolylpyrrolecarboxamides as protein kinase inhibitors
IN Tang, Qing; Maltais, Francois; Janetka, James Walter; Hale, Michael Robin
PA Vertex Pharmaceuticals Incorporated, USA
SO PCT Int. Appl., 66 pp.
CODEN: PIXXD2
DT Patent
LA English
IC ICM C07D401-04
ICS C07D405-14; C07D401-14; C07D403-14; C07D413-14; A61K031-4155; A61K031-4439; A61P035-00; A61P029-00
CC 28-8 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2003011854	A1	20030213	WO 2002-US24723	20020802

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG,

CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
US 2003139452 A1 20030724 US 2002-212292 20020802
PRAI US 2001-309886P P 20010803
OS MARPAT 138:153530
GI



I

AB Title compds. [I; B = substituted aryl, heteroaryl, heterocyclyl; Q = (substituted) alkylidene; n = 0, 1; R1 = H, F, R, N(R7)2, OR7, NR7COR7, NR7SO2R7, etc.; R3 = H, R, OH, OR, N(R7)2, F, cyano; R4 = (CH2)yR6, N(R5)2, etc.; R = (substituted) aliph., aryl, heteroaryl, heterocyclyl; R5 = R, (CH2)yR6, R7, CON(R7)2, SO2R7, etc.; y = 0-6; R6 = H, R, (CH2)yR, OH, OR, CO2R, N(R7)2, etc.; R7 = H, (substituted) aliph.; N(R7)2 = 5-8 membered heterocyclyl, heteroaryl], were prepd. Thus, Ac-hydroxyproline-OH was stirred with HOBT and EDCI in DMF; 4-[4-(4-aminomethyl-3-chlorophenyl)-1H-pyrazol-3-yl]-1H-pyrrole-2-carboxylic acid [1-(3-chloro-4-fluorophenyl)-2-hydroxyethyl]amide (prepn. given) and triethylamine were added followed by stirring for 2 h to give 4-[4-[4-[[(1-acetyl-4-hydroxypyrrolidine-2-carbonyl)amino]methyl]-3-chlorophenyl]-1H-pyrazol-3-yl]-1H-pyrrole-2-carboxylic acid [1-(3-chloro-4-fluorophenyl)-2-hydroxyethyl]amide. The latter inhibited ERK2 with Ki<1 .mu.M. I are useful for treating disease states in mammals that are alleviated by a protein kinase inhibitor, particularly diseases such as cancer, inflammatory disorders, restenosis, and cardiovascular disease.

ST pyrazolylpyrrolecarboxamide prepn protein kinase inhibitor; ERK2 AKT kinase inhibitor pyrazolylpyrrolecarboxamide prepn; cancer diabetes hepatomegaly cardiovascular disease treatment; alzheimers disease cystic fibrosis viral disease treatment pyrazolylpyrrolecarboxamide

IT Lung, neoplasm
(adenocarcinoma, treatment; prepn. of pyrazolylpyrrolecarboxamides as protein kinase inhibitors)

IT Platelet (blood)
(aggregation, treatment; prepn. of pyrazolylpyrrolecarboxamides as protein kinase inhibitors)

IT Nervous system, disease
(amyotrophic lateral sclerosis, treatment; prepn. of pyrazolylpyrrolecarboxamides as protein kinase inhibitors)

IT Antiarteriosclerotics
(antiatherosclerotics; prepn. of pyrazolylpyrrolecarboxamides as protein kinase inhibitors)

IT Bladder, neoplasm
(carcinoma, treatment; prepn. of pyrazolylpyrrolecarboxamides as protein kinase inhibitors)
IT Nervous system, disease
Nervous system, neoplasm
(central, treatment; prepn. of pyrazolylpyrrolecarboxamides as protein kinase inhibitors)
IT Uterus, neoplasm
(cervix, treatment; prepn. of pyrazolylpyrrolecarboxamides as protein kinase inhibitors)
IT Leukemia
(chronic myelocytic, treatment; prepn. of pyrazolylpyrrolecarboxamides as protein kinase inhibitors)
IT Intestine, neoplasm
(colon, treatment; prepn. of pyrazolylpyrrolecarboxamides as protein kinase inhibitors)
IT Intestine, neoplasm
(colorectal, treatment; prepn. of pyrazolylpyrrolecarboxamides as protein kinase inhibitors)
IT Artery, disease
(coronary, restenosis, treatment; prepn. of pyrazolylpyrrolecarboxamides as protein kinase inhibitors)
IT Urogenital tract
(disease, cancer treatment; prepn. of pyrazolylpyrrolecarboxamides as protein kinase inhibitors)
IT Immunity
(disorder, treatment; prepn. of pyrazolylpyrrolecarboxamides as protein kinase inhibitors)
IT Thyroid gland, neoplasm
(follicular cell carcinoma, treatment; prepn. of pyrazolylpyrrolecarboxamides as protein kinase inhibitors)
IT Neuroglia, neoplasm
(glioblastoma, treatment; prepn. of pyrazolylpyrrolecarboxamides as protein kinase inhibitors)
IT Leukemia
(hairy-cell, treatment; prepn. of pyrazolylpyrrolecarboxamides as protein kinase inhibitors)
IT Liver, disease
(hepatomegaly, treatment; prepn. of pyrazolylpyrrolecarboxamides as protein kinase inhibitors)
IT Heart, disease
(hypertrophy, treatment; prepn. of pyrazolylpyrrolecarboxamides as protein kinase inhibitors)
IT Heart, disease
(infarction, treatment; prepn. of pyrazolylpyrrolecarboxamides as protein kinase inhibitors)
IT Brain, disease
(ischemia, treatment; prepn. of pyrazolylpyrrolecarboxamides as protein kinase inhibitors)
IT Skin, neoplasm
(**keratoacanthoma**, treatment; prepn. of pyrazolylpyrrolecarboxamides as protein kinase inhibitors)
IT Lung, neoplasm
(large-cell carcinoma, treatment; prepn. of pyrazolylpyrrolecarboxamides as protein kinase inhibitors)
IT Hematopoietic precursor cell
(myeloid, cancer treatment; prepn. of pyrazolylpyrrolecarboxamides as protein kinase inhibitors)

IT Nerve, neoplasm
(neuroblastoma, treatment; prepn. of pyrazolylpyrrolecarboxamides as protein kinase inhibitors)
IT Thyroid gland, neoplasm
(papillary carcinoma, treatment; prepn. of pyrazolylpyrrolecarboxamides as protein kinase inhibitors)
IT Allergy inhibitors
Anti-Alzheimer's agents
Anti-infective agents
Anti-inflammatory agents
Antitumor agents
Human
Platelet aggregation inhibitors
(prepn. of pyrazolylpyrrolecarboxamides as protein kinase inhibitors)
IT Kidney, neoplasm
(renal cell carcinoma, treatment; prepn. of pyrazolylpyrrolecarboxamides as protein kinase inhibitors)
IT Testis, neoplasm
(seminoma, treatment; prepn. of pyrazolylpyrrolecarboxamides as protein kinase inhibitors)
IT Lung, neoplasm
(small-cell carcinoma, treatment; prepn. of pyrazolylpyrrolecarboxamides as protein kinase inhibitors)
IT Carcinoma
(squamous cell, treatment; prepn. of pyrazolylpyrrolecarboxamides as protein kinase inhibitors)
IT Brain, disease
(stroke, treatment; prepn. of pyrazolylpyrrolecarboxamides as protein kinase inhibitors)
IT Adenoma
Allergy
Alzheimer's disease
Antiviral agents
Atherosclerosis
Autoimmune disease
Biliary tract, neoplasm
Bone, disease
Bone, neoplasm
Brain, neoplasm
Cardiovascular system, disease
Cell death
Cystic fibrosis
Diabetes mellitus
Endocrine system, disease
Esophagus, neoplasm
Hodgkin's disease
Immunodeficiency
Infection
Inflammation
Intestine, neoplasm
Larynx, neoplasm
Leukemia
Liver, disease
Liver, neoplasm
Lung, neoplasm
Lymphoma
Mammary gland, neoplasm
Melanoma

Mouth, neoplasm
Neoplasm
Nervous system, disease
Ovary, neoplasm
Pancreas, neoplasm
Pharynx, neoplasm
Prostate gland, neoplasm
Psoriasis
Sarcoma
Skin, neoplasm
Stomach, neoplasm
Testis, neoplasm
Thyroid gland, neoplasm
Transplant and Transplantation
(treatment; prepn. of pyrazolylpyrrolecarboxamides as protein kinase inhibitors)

IT Carcinoma
(undifferentiated, treatment; prepn. of pyrazolylpyrrolecarboxamides as protein kinase inhibitors)

IT 137632-08-7, Erk2 kinase 148640-14-6
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(inhibitors; prepn. of pyrazolylpyrrolecarboxamides as protein kinase inhibitors)

IT 496856-34-9P 496856-35-0P 496856-36-1P 496856-37-2P 496856-38-3P
496856-39-4P 496856-40-7P **496856-41-8P** 496856-42-9P
496856-43-0P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of pyrazolylpyrrolecarboxamides as protein kinase inhibitors)

IT 5414-19-7, 2-Bromoethyl ether 7216-42-4, 4-Pyridinecarboxaldehyde N-oxide 33697-81-3, 3-Chloro-4-hydroxyphenylacetic acid 33996-33-7, N-Acetylhydroxyproline 35302-72-8, 2-(Trichloroacetyl)pyrrole 496856-51-0 496856-52-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of pyrazolylpyrrolecarboxamides as protein kinase inhibitors)

IT 57017-95-5P, Methyl 3-chloro-4-hydroxyphenylacetate 496856-44-1P
496856-45-2P 496856-46-3P 496856-47-4P 496856-48-5P 496856-49-6P
496856-50-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of pyrazolylpyrrolecarboxamides as protein kinase inhibitors)

RE.CNT 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE
(1) Ambiter; Screening Collection (Catalog) 1999
(2) Anantanarayan; US 5932576 A 1999 HCAPLUS
(3) Davis; US 5922741 A 1999 HCAPLUS
(4) G D Searle & Co; WO 9852941 A 1998 HCAPLUS
(5) Vertex Pharmaceuticals; WO 0156993 A 2001 HCAPLUS
(6) Vertex Pharmaceuticals; WO 0157022 A 2001 HCAPLUS
(7) Vertex Pharmaceuticals; WO 0222610 A 2002 HCAPLUS

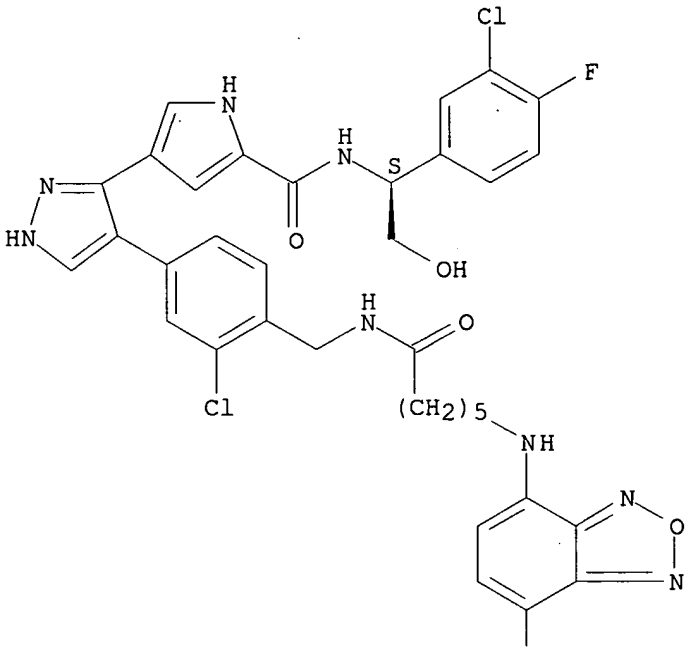
IT **496856-41-8P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of pyrazolylpyrrolecarboxamides as protein kinase inhibitors)

RN 496856-41-8 HCAPLUS
CN 1H-Pyrrole-2-carboxamide, N-[(1S)-1-(3-chloro-4-fluorophenyl)-2-

hydroxyethyl]-4-[4-[3-chloro-4-[[[6-[(7-nitro-2,1,3-benzoxadiazol-4-yl)amino]-1-oxohexyl]amino]methyl]phenyl]-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

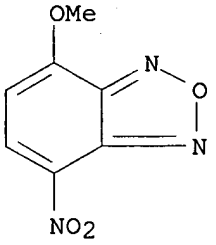


PAGE 2-A

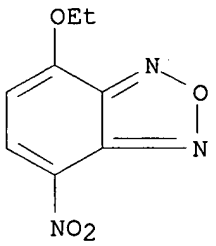
L32 ANSWER 2 OF 9 HCAPLUS COPYRIGHT 2003 ACS on STN
AN 2002:733871 HCAPLUS
DN 137:252675
TI Two-component direct **hair** dyes
IN Umbricht, Gisela; Braun, Hans-Juergen; Oberson, Sylviane; Mueller, Catherine
PA Wella AG, Germany
SO Ger. Offen., 12 pp.
CODEN: GWXXBX
DT Patent
LA German
IC ICM A61K007-13
CC 62-3 (Essential Oils and Cosmetics)
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	DE 10114426	A1	20020926	DE 2001-10114426	20010324

PRAI DE 2001-10114426 20010324
OS MARPAT 137:252675
AB The invention concerns direct **hair** dyes that are composed of two dyes; component A1 contains benzodiazole, benzothiazole, benzoselenadiazole derivs.; component A2 is selected from the group of aliph. esters, indolium, quinolinium, pyrazole, pyrazolinone, furan, etc. derivs. Thus component A1 contained (g): 7-chloro-4-nitro-2,1,3-benzoxadiazole 0.25; ethanol 5.00; Plantaren 2000 4.00; EDTA disodium hydrate 0.20; water to 100. Component A2 was 0.22 g 1-phenyl-3-methyl-5-pyrazolone. The components were mixed and sodium carbonate was added; the pH was set to desired value with sodium hydroxide and the mixt. was applied to **hair**.
ST direct **hair** dye two component sodium carbonate
IT pH
(two-component direct **hair** dyes)
IT 59-48-3, Oxindole 67-52-7, Barbituric acid 89-25-8, 1-Phenyl-3-methyl-5-pyrazolone 105-34-0, Acetic acid, cyano-, methyl ester 105-53-3, Malonic acid diethyl ester 105-56-6, Acetic acid, cyano-, ethyl ester 107-91-5, 2-Cyanoacetamide 108-26-9 108-59-8, Malonic acid dimethyl ester 109-77-3, Malonic acid dinitrile 118-12-7, 1,3,3-Trimethyl-2-methyleneindoline 141-84-4, Rhodanine 372-09-8 497-19-8, Sodium carbonate, biological studies 504-02-9, Cyclohexane-1,3-dione 504-17-6, Thiobarbituric acid 541-50-4D, Acetoacetic acid, esters 553-86-6, Cumaranone 606-23-5, 1,3-Indandione 606-55-3 608-08-2, 3-Indoxylacetate 876-87-9 939-83-3 1753-20-4 2160-10-3 2207-29-6 2274-63-7 2274-89-7 2654-52-6 2749-59-9 2785-06-0 3158-63-2, 1,3-Dimethylthiobarbituric acid 3524-07-0 5418-63-3, 1,2,3,3-Tetramethyl-3H-indoliumiodide 5714-17-0 5718-83-2, Rhodanine-3-acetic acid 6583-06-8 10199-89-0, 7-Chloro-4-nitro-2,1,3-benzoxadiazole 15639-38-0 15639-43-7 15944-78-2 16322-19-3, 4-Nitro-2,1,3-benzoxadiazole 16859-86-2, 1,4-Dimethylquinoliniumiodide 18333-71-6 **18333-73-8**, 2,1,3-Benzoxadiazole, 4-methoxy-7-nitro- 18378-23-9 18392-74-0 18392-77-3 18453-42-4 19951-28-1 19951-33-8 19951-34-9 20718-28-9 20718-41-6 20718-46-1 20718-47-2 20718-48-3 26460-78-6 26738-24-9 29270-56-2, 2,1,3-Benzoxadiazole, 4-fluoro-7-nitro- 30536-22-2 32051-92-6 35128-56-4, 2,1,3-Benzoxadiazole, 4-bromo-7-nitro- 41927-50-8 52120-98-6 59997-51-2, Pivaloylacetonitrile 61224-35-9, 1,2,3,3-Tetramethyl-3H-indolium-p-toluene sulfonate 68579-76-0 70264-71-0 72023-79-1 **81432-10-2**, 2,1,3-Benzoxadiazole, 4-ethoxy-7-nitro- 89365-28-6 89365-31-1 89365-32-2 89793-80-6 89793-88-4 90841-38-6 91267-92-4 91330-69-7 91760-88-2 100181-80-4 125292-42-4 131202-67-0 131202-71-6 227199-11-3 257932-06-2 257932-07-3 404839-62-9 404839-63-0 404839-64-1 413612-09-6 460987-45-5 460987-46-6 460987-47-7 460987-48-8 460987-49-9 460987-50-2 460987-52-4
RL: COS (Cosmetic use); BIOL (Biological study); USES (Uses)
(two-component direct **hair** dyes)
IT **18333-73-8**, 2,1,3-Benzoxadiazole, 4-methoxy-7-nitro-
81432-10-2, 2,1,3-Benzoxadiazole, 4-ethoxy-7-nitro-
RL: COS (Cosmetic use); BIOL (Biological study); USES (Uses)
(two-component direct **hair** dyes)
RN 18333-73-8 HCAPLUS
CN 2,1,3-Benzoxadiazole, 4-methoxy-7-nitro- (9CI) (CA INDEX NAME)



RN 81432-10-2 HCAPLUS
CN 2,1,3-Benzoxadiazole, 4-ethoxy-7-nitro- (9CI) (CA INDEX NAME)



L32 ANSWER 3 OF 9 HCAPLUS COPYRIGHT 2003 ACS on STN
AN 2002:220344 HCAPLUS
DN 136:267892
TI Use of 4-nitro-2,1,3-benzoxadiazole derivatives as **hair** dyes
IN Pasquier, Cecile; Charriere, Veronique; Braun, Hans-Juergen
PA Wella Aktiengesellschaft, Germany
SO PCT Int. Appl., 35 pp.
CODEN: PIXXD2
DT Patent
LA German
IC ICM A61K007-13
CC 62-3 (Essential Oils and Cosmetics)
Section cross-reference(s): 27, 41

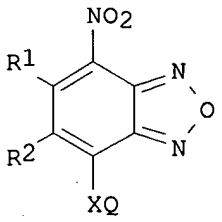
applicant

FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2002022094	A1	20020321	WO 2001-EP7497	20010629
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
DE 10045599	A1	20020404	DE 2000-10045599	20000915
AU 2001069112	A5	20020326	AU 2001-69112	20010629
BR 2001007208	A	20020709	BR 2001-7208	20010629
EP 1317242	A1	20030611	EP 2001-947431	20010629

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR

US 2002189032 A1 20021219 US 2002-89207 20020326
PRAI DE 2000-10045599 A 20000915
WO 2001-EP7497 W 20010629
OS MARPAT 136:267892
GI



I

AB The invention relates to the use of 4-nitro-benzo-2,1,3-oxadiazol derivs. of general formula (I) as dyes in coloring agents for **keratin** fibers, for example, **wool**, **silk**, **fur** or **hair** and particularly human **hair**. In formula I X represents oxygen, sulfur or NRa, Ra represents hydrogen, an (C1-C4) alkyl group, a monohydroxy (C1-C4) alkyl group, a polyhydroxy (C2-C4) alkyl group, a mono (C1-C4) alkoxy (C1-C4) alkyl group; R1 and R2 can be identical or different and represent independently from each other hydrogen, a halogen atom, an (C1-C4) alkyl group, an (C1-C4) alkyl group substituted by a halogen atom, an (C1-C4) alkoxy group, a nitro group or a NRbRc group, wherein the radicals Rb and Rc can be identical or different and represent independently from each other hydrogen, a (C1-C4) alkyl group, an optionally substituted arom. carbocycle or an (C1-C4) alkane carbonyl group, or Rb and Rc together with the nitrogen atom form a heterocyclic (C3-C6) group; Q represents hydrogen, an aliph. group, an arom. isocyclic group or an arom. heterocyclic group. Thus 7-nitro-4-(N-phenyl-amino)-2,1,3-benzodioxazole was synthesized and 2.5 mmol were used in a **hair** dye that further contained (g): ethanol 5; Plantaren 2000 4.0; EDTA sodium salt hydrate 0.2; water to 100.

ST nitro benzoxadiazole deriv **hair** dye

IT **Hair** preparations
(dyes; use of 4-nitro-2,1,3-benzoxadiazole derivs. as **hair** dyes)

IT **Fur**
Silk
Wool
(use of 4-nitro-2,1,3-benzoxadiazole derivs. as **hair** dyes)

IT **Keratins**
RL: COS (Cosmetic use); BIOL (Biological study); USES (Uses)
(use of 4-nitro-2,1,3-benzoxadiazole derivs. as **hair** dyes)

IT **1455-87-4** 7722-84-1, Hydrogen peroxide, biological studies
10199-91-4, 4-Amino-7-nitro-2, 1,3-benzoxadiazole
16322-23-9 18378-17-1 18378-18-2
19155-64-7 53619-61-7 53619-62-8
53619-63-9 53619-64-0 73853-83-5
73853-84-6 81432-10-2 90786-92-8

90786-95-1 97346-17-3 101237-21-2
101237-22-3 101237-23-4 101237-24-5
101237-27-8 102565-92-4 118025-13-1
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199727-71-4 324525-87-3 404823-74-1
404823-79-6 404823-80-9 404823-81-0
404823-86-5 404823-87-6 404823-88-7
404823-89-8
RL: COS (Cosmetic use); BIOL (Biological study); USES (Uses)
(use of 4-nitro-2,1,3-benzoxadiazole derivs. as **hair** dyes)

IT **16597-10-7P 18333-73-8P 18378-15-9P**
101237-25-6P 101237-26-7P 404823-73-0P
RL: COS (Cosmetic use); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(use of 4-nitro-2,1,3-benzoxadiazole derivs. as **hair** dyes)

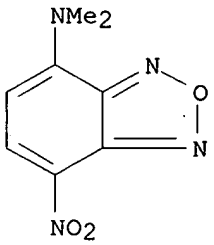
IT 62-53-3, Aniline, reactions 106-50-3, 1,4-Diaminobenzene, reactions 108-95-2, Phenol, reactions 123-30-8, 4-Aminophenol 10199-89-0, 4-Chloro-7-nitro-2,1,3-benzoxadiazole 93841-25-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(use of 4-nitro-2,1,3-benzoxadiazole derivs. as **hair** dyes)

RE.CNT 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD

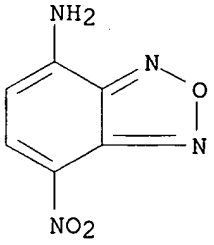
RE
(1) Akademie der Wissenschaften der Ddr; DE 277678 C
(2) Bachmann, H; US 4620850 A 1986 HCAPLUS
(3) Henkel; WO 0147485 A 2001
(4) Lim, M; US 5055110 A 1991 HCAPLUS
(5) M Luther Universitat; DD 228900 A 1985 HCAPLUS

IT **1455-87-4 10199-91-4**, 4-Amino-7-nitro-2,1,3-benzoxadiazole **16322-23-9 18378-17-1**
18378-18-2 19155-64-7 53619-61-7
53619-62-8 53619-63-9 53619-64-0
73853-83-5 73853-84-6 81432-10-2
90786-92-8 90786-95-1 97346-17-3
101237-21-2 101237-22-3 101237-23-4
101237-24-5 101237-27-8 102565-92-4
118025-13-1 121782-85-2 121782-87-4
121782-88-5 121782-92-1 121782-93-2
126865-59-6 126865-60-9 126865-61-0
126865-63-2 155866-58-3 199727-69-0
199727-70-3 199727-71-4 324525-87-3
404823-74-1 404823-79-6 404823-80-9
404823-81-0 404823-86-5 404823-87-6
404823-88-7 404823-89-8
RL: COS (Cosmetic use); BIOL (Biological study); USES (Uses)
(use of 4-nitro-2,1,3-benzoxadiazole derivs. as **hair** dyes)

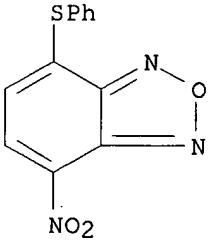
RN 1455-87-4 HCAPLUS
CN 2,1,3-Benzoxadiazol-4-amine, N,N-dimethyl-7-nitro- (9CI) (CA INDEX NAME)



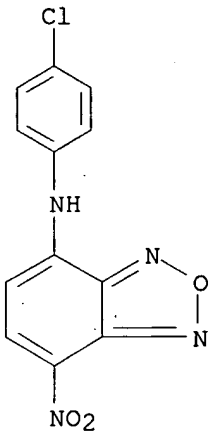
RN 10199-91-4 HCAPLUS
CN 2,1,3-Benzoxadiazol-4-amine, 7-nitro- (9CI) (CA INDEX NAME)



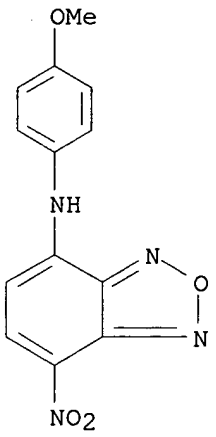
RN 16322-23-9 HCAPLUS
CN 2,1,3-Benzoxadiazole, 4-nitro-7-(phenylthio)- (9CI) (CA INDEX NAME)



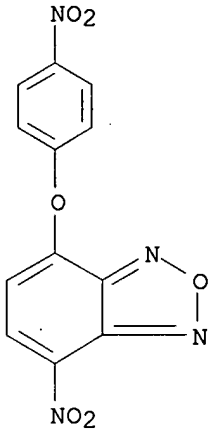
RN 18378-17-1 HCAPLUS
CN 2,1,3-Benzoxadiazol-4-amine, N-(4-chlorophenyl)-7-nitro- (9CI) (CA INDEX NAME)



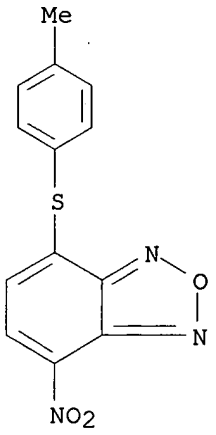
RN 18378-18-2 HCAPLUS
CN 2,1,3-Benzoxadiazol-4-amine, N-(4-methoxyphenyl)-7-nitro- (9CI) (CA INDEX NAME)



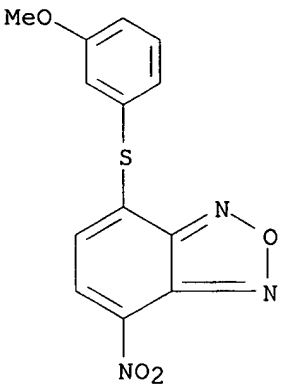
RN 19155-64-7 HCAPLUS
CN 2,1,3-Benzoxadiazole, 4-nitro-7-(4-nitrophenoxy)- (9CI) (CA INDEX NAME)



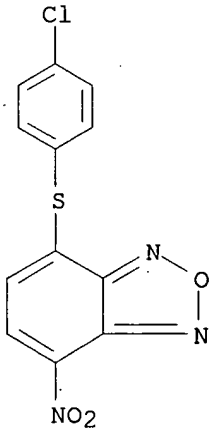
RN 53619-61-7 HCAPLUS
CN 2,1,3-Benzoxadiazole, 4-[(4-methylphenyl)thio]-7-nitro- (9CI) (CA INDEX NAME)



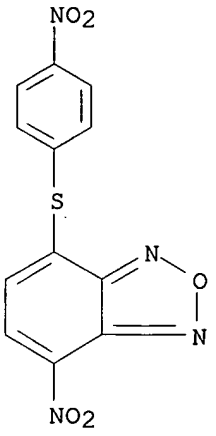
RN 53619-62-8 HCAPLUS
CN 2,1,3-Benzoxadiazole, 4-[(3-methoxyphenyl)thio]-7-nitro- (9CI) (CA INDEX NAME)



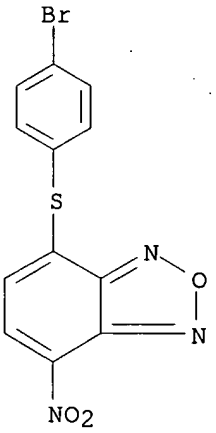
RN 53619-63-9 HCAPLUS
CN 2,1,3-Benzoxadiazole, 4-[(4-chlorophenyl)thio]-7-nitro- (9CI) (CA INDEX NAME)



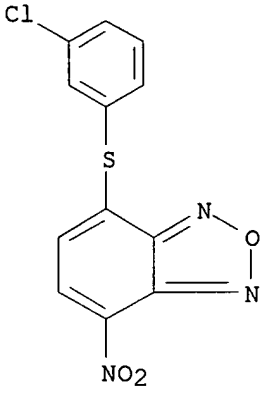
RN 53619-64-0 HCAPLUS
CN 2,1,3-Benzoxadiazole, 4-nitro-7-[(4-nitrophenyl)thio]- (9CI) (CA INDEX NAME)



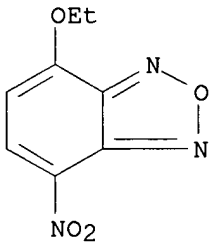
RN 73853-83-5 HCAPLUS
CN 2,1,3-Benzoxadiazole, 4-[(4-bromophenyl)thio]-7-nitro- (9CI) (CA INDEX NAME)



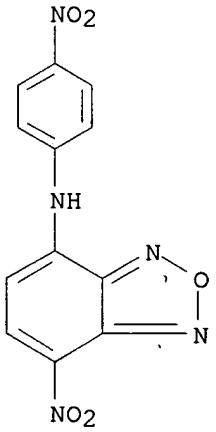
RN 73853-84-6 HCAPLUS
CN 2,1,3-Benzoxadiazole, 4-[(3-chlorophenyl)thio]-7-nitro- (9CI) (CA INDEX NAME)



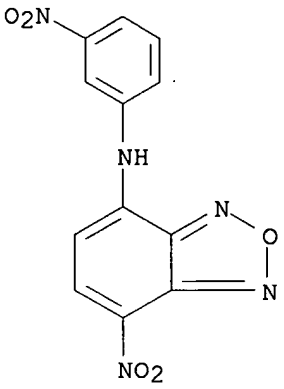
RN 81432-10-2 HCAPLUS
CN 2,1,3-Benzoxadiazole, 4-ethoxy-7-nitro- (9CI) (CA INDEX NAME)



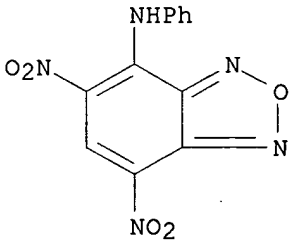
RN 90786-92-8 HCAPLUS
CN 2,1,3-Benzoxadiazol-4-amine, 7-nitro-N-(4-nitrophenyl)- (9CI) (CA INDEX NAME)



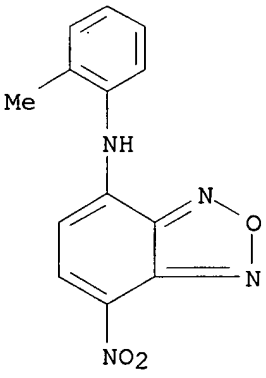
RN 90786-95-1 HCAPLUS
CN 2,1,3-Benzoxadiazol-4-amine, 7-nitro-N-(3-nitrophenyl)- (9CI) (CA INDEX NAME)



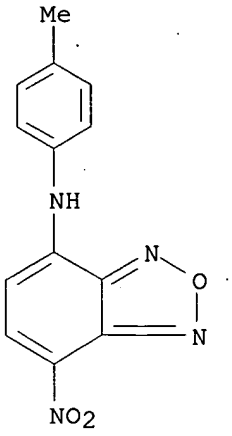
RN 97346-17-3 HCAPLUS
CN 2,1,3-Benzoxadiazol-4-amine, 5,7-dinitro-N-phenyl- (9CI) (CA INDEX NAME)



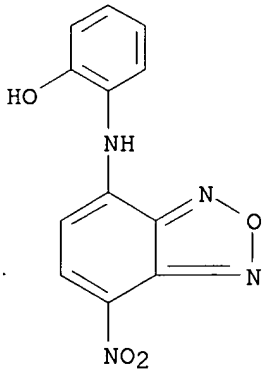
RN 101237-21-2 HCAPLUS
CN 2,1,3-Benzoxadiazol-4-amine, N-(2-methylphenyl)-7-nitro- (9CI) (CA INDEX NAME)



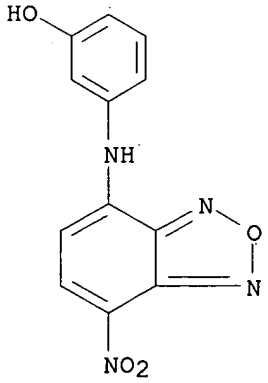
RN 101237-22-3 HCAPLUS
CN 2,1,3-Benzoxadiazol-4-amine, N-(4-methylphenyl)-7-nitro- (9CI) (CA INDEX NAME)



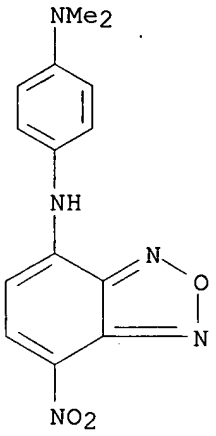
RN 101237-23-4 HCAPLUS
CN Phenol, 2-[(7-nitro-2,1,3-benzoxadiazol-4-yl)amino]- (9CI) (CA INDEX NAME)



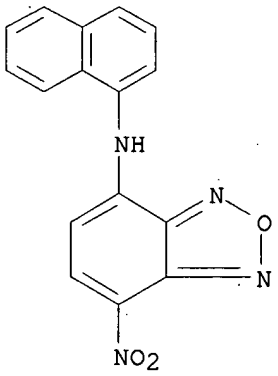
RN 101237-24-5 HCAPLUS
CN Phenol, 3-[(7-nitro-2,1,3-benzoxadiazol-4-yl)amino]- (9CI) (CA INDEX NAME)



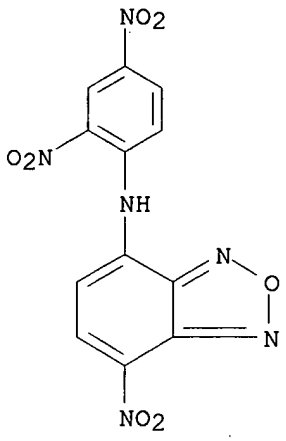
RN 101237-27-8 HCAPLUS
CN 1,4-Benzenediamine, N,N-dimethyl-N'-(7-nitro-2,1,3-benzoxadiazol-4-yl)-(9CI) (CA INDEX NAME)



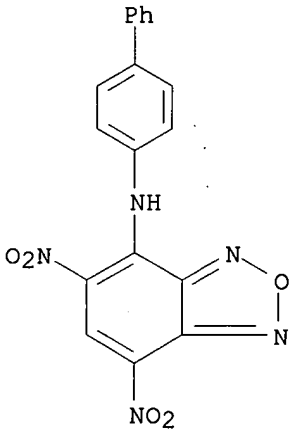
RN 102565-92-4 HCAPLUS
CN 2,1,3-Benzoxadiazol-4-amine, N-1-naphthalenyl-7-nitro- (9CI) (CA INDEX NAME)



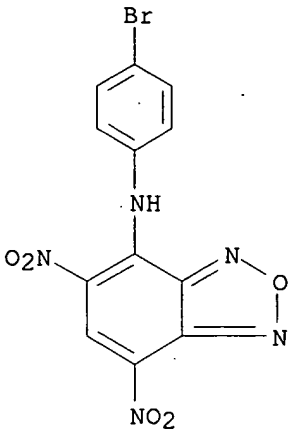
RN 118025-13-1 HCAPLUS
CN 2,1,3-Benzoxadiazol-4-amine, N-(2,4-dinitrophenyl)-7-nitro- (9CI) (CA INDEX NAME)



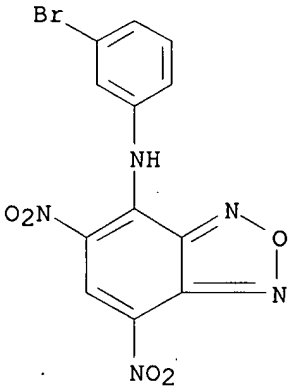
RN 121782-85-2 HCAPLUS
CN 2,1,3-Benzoxadiazol-4-amine, N-[1,1'-biphenyl]-4-yl-5,7-dinitro- (9CI) (CA INDEX NAME)



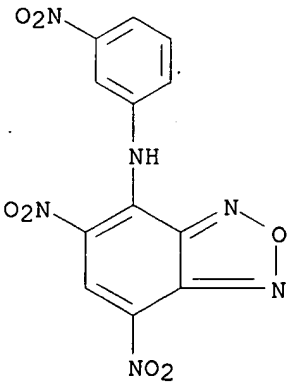
RN 121782-87-4 HCAPLUS
CN 2,1,3-Benzoxadiazol-4-amine, N-(4-bromophenyl)-5,7-dinitro- (9CI) (CA INDEX NAME)



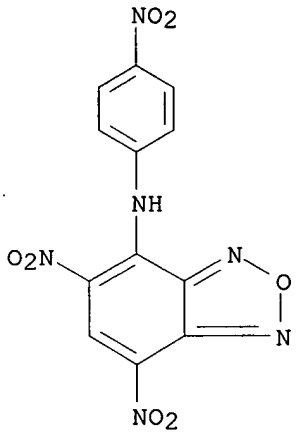
RN 121782-88-5 HCAPLUS
CN 2,1,3-Benzoxadiazol-4-amine, N-(3-bromophenyl)-5,7-dinitro- (9CI) (CA INDEX NAME)



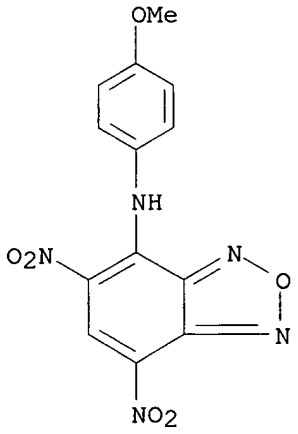
RN 121782-92-1 HCAPLUS
CN 2,1,3-Benzoxadiazol-4-amine, 5,7-dinitro-N-(3-nitrophenyl)- (9CI) (CA INDEX NAME)



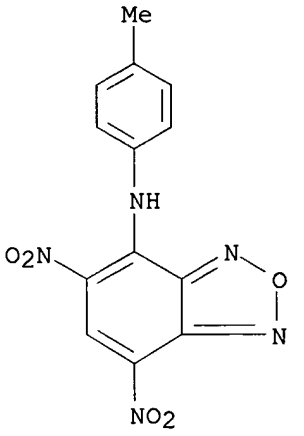
RN 121782-93-2 HCAPLUS
CN 2,1,3-Benzoxadiazol-4-amine, 5,7-dinitro-N-(4-nitrophenyl)- (9CI) (CA INDEX NAME)



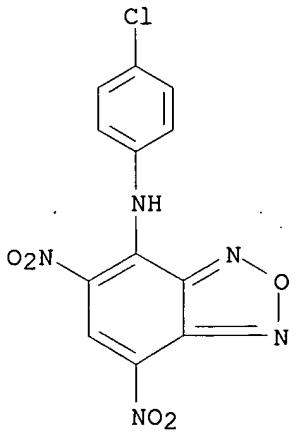
RN 126865-59-6 HCAPLUS
CN 2,1,3-Benzoxadiazol-4-amine, N-(4-methoxyphenyl)-5,7-dinitro- (9CI) (CA INDEX NAME)



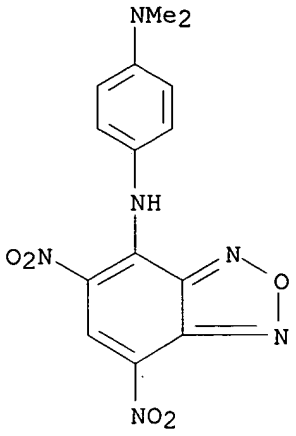
RN 126865-60-9 HCAPLUS
CN 2,1,3-Benzoxadiazol-4-amine, N-(4-methylphenyl)-5,7-dinitro- (9CI) (CA INDEX NAME)



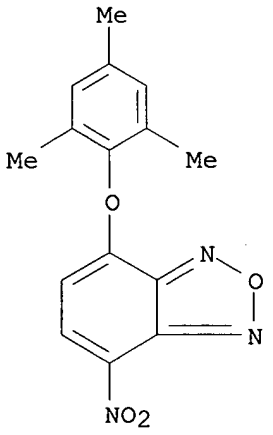
RN 126865-61-0 HCAPLUS
CN 2,1,3-Benzoxadiazol-4-amine, N-(4-chlorophenyl)-5,7-dinitro- (9CI) (CA INDEX NAME)



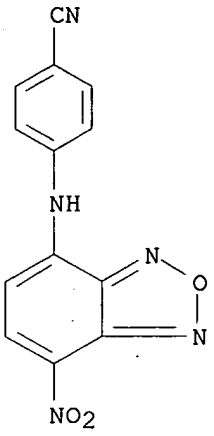
RN 126865-63-2 HCAPLUS
CN 1,4-Benzenediamine, N'-(5,7-dinitro-2,1,3-benzoxadiazol-4-yl)-N,N-dimethyl- (9CI) (CA INDEX NAME)



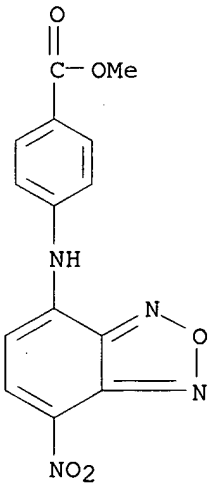
RN 155866-58-3 HCAPLUS
CN 2,1,3-Benzoxadiazole, 4-nitro-7-(2,4,6-trimethylphenoxy)- (9CI) (CA INDEX NAME)



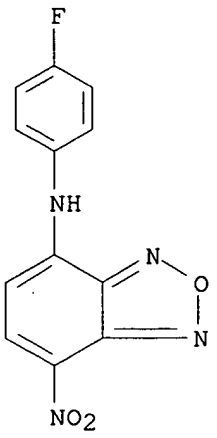
RN 199727-69-0 HCAPLUS
CN Benzonitrile, 4-[(7-nitro-2,1,3-benzoxadiazol-4-yl)amino]- (9CI) (CA INDEX NAME)



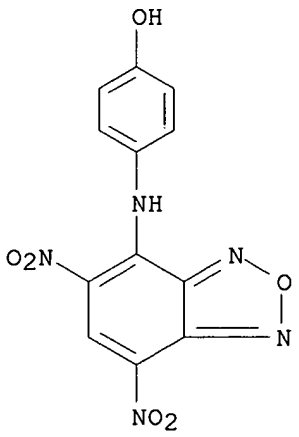
RN 199727-70-3 HCAPLUS
CN Benzoic acid, 4-[(7-nitro-2,1,3-benzoxadiazol-4-yl)amino]-, methyl ester (9CI) (CA INDEX NAME)



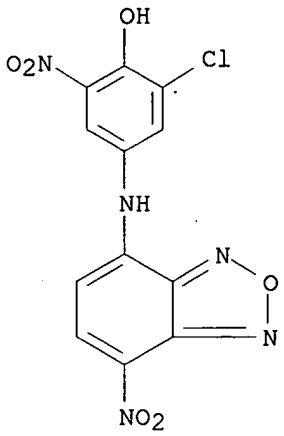
RN 199727-71-4 HCAPLUS
CN 2,1,3-Benzoxadiazol-4-amine, N-(4-fluorophenyl)-7-nitro- (9CI) (CA INDEX NAME)



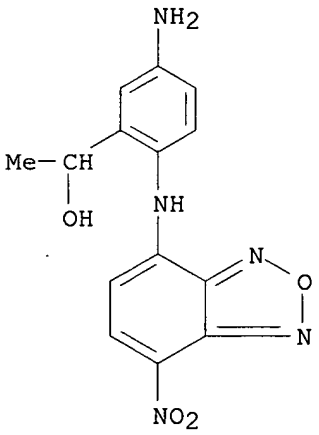
RN 324525-87-3 HCAPLUS
CN Phenol, 4-[(5,7-dinitro-2,1,3-benzoxadiazol-4-yl)amino]- (9CI) (CA INDEX NAME)



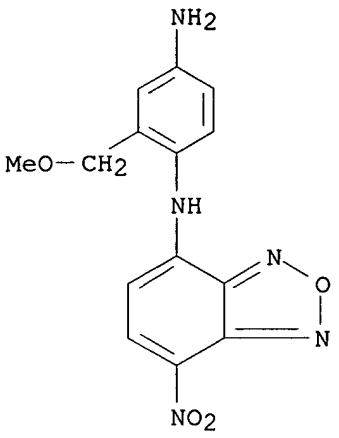
RN 404823-74-1 HCAPLUS
CN Phenol, 2-chloro-6-nitro-4-[(7-nitro-2,1,3-benzoxadiazol-4-yl)amino]- (9CI) (CA INDEX NAME)



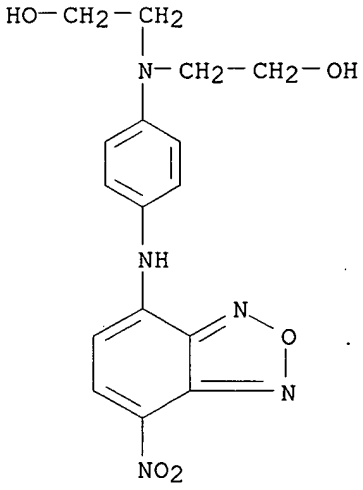
RN 404823-79-6 HCAPLUS
CN Benzenemethanol, 5-amino-.alpha.-methyl-2-[(7-nitro-2,1,3-benzoxadiazol-4-yl)amino]- (9CI) (CA INDEX NAME)



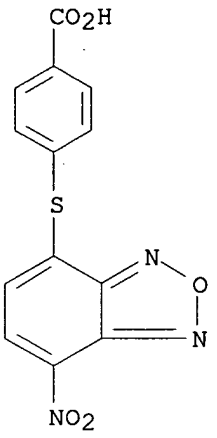
RN 404823-80-9 HCAPLUS
CN 1,4-Benzenediamine, 2-(methoxymethyl)-N1-(7-nitro-2,1,3-benzoxadiazol-4-yl)- (9CI) (CA INDEX NAME)



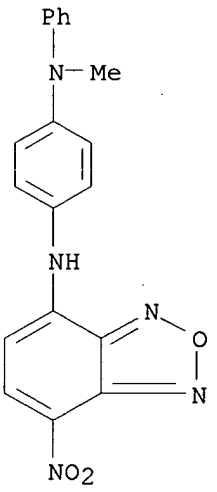
RN 404823-81-0 HCAPLUS
CN Ethanol, 2,2'-[[4-[(7-nitro-2,1,3-benzoxadiazol-4-yl)amino]phenyl]imino]bis- (9CI) (CA INDEX NAME)



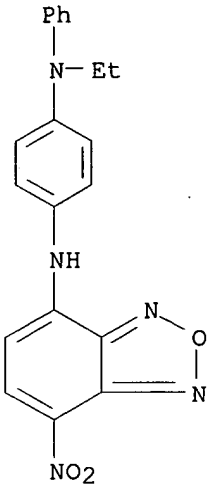
RN 404823-86-5 HCAPLUS
CN Benzoic acid, 4-[(7-nitro-2,1,3-benzoxadiazol-4-yl)thio]- (9CI) (CA INDEX NAME)



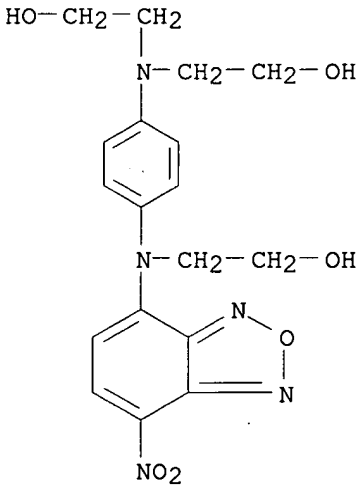
RN 404823-87-6 HCAPLUS
CN 1,4-Benzenediamine, N-methyl-N'-(7-nitro-2,1,3-benzoxadiazol-4-yl)-N-phenyl- (9CI) (CA INDEX NAME)



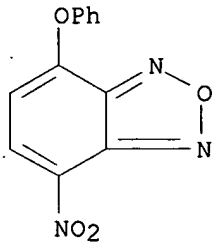
RN 404823-88-7 HCAPLUS
CN 1,4-Benzenediamine, N-ethyl-N'-(7-nitro-2,1,3-benzoxadiazol-4-yl)-N-phenyl- (9CI) (CA INDEX NAME)



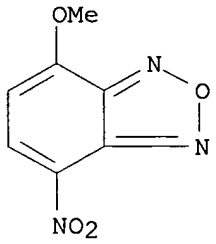
RN 404823-89-8 HCAPLUS
CN Ethanol, 2,2'-[[4-[(2-hydroxyethyl)(7-nitro-2,1,3-benzoxadiazol-4-yl)amino]phenyl]imino]bis- (9CI) (CA INDEX NAME)



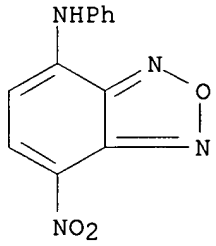
IT **16597-10-7P 18333-73-8P 18378-15-9P**
101237-25-6P 101237-26-7P 404823-73-0P
RL: COS (Cosmetic use); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(use of 4-nitro-2,1,3-benzoxadiazole derivs. as **hair** dyes)
RN 16597-10-7 HCAPLUS
CN 2,1,3-Benzoxadiazole, 4-nitro-7-phenoxy- (9CI) (CA INDEX NAME)



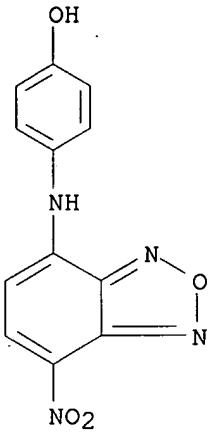
RN 18333-73-8 HCAPLUS
CN 2,1,3-Benzoxadiazole, 4-methoxy-7-nitro- (9CI) (CA INDEX NAME)



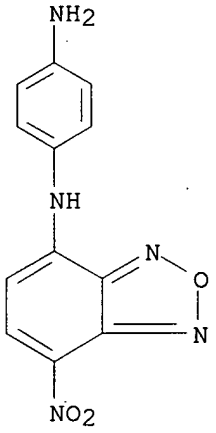
RN 18378-15-9 HCAPLUS
CN 2,1,3-Benzoxadiazol-4-amine, 7-nitro-N-phenyl- (9CI) (CA INDEX NAME)



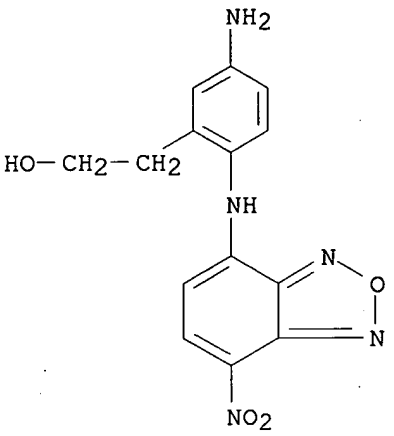
RN 101237-25-6 HCAPLUS
CN Phenol, 4-[(7-nitro-2,1,3-benzoxadiazol-4-yl)amino]- (9CI) (CA INDEX NAME)



RN 101237-26-7 HCAPLUS
CN 1,4-Benzenediamine, N-(7-nitro-2,1,3-benzoxadiazol-4-yl)- (9CI) (CA INDEX NAME)



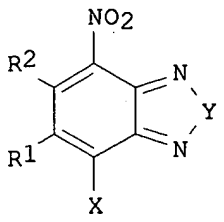
RN 404823-73-0 HCAPLUS
CN Benzeneethanol, 5-amino-2-[(7-nitro-2,1,3-benzoxadiazol-4-yl)amino]- (9CI) (CA INDEX NAME)



L32 ANSWER 4 OF 9 HCAPLUS COPYRIGHT 2003 ACS on STN
AN 2002:220343 HCAPLUS
DN 136:267891
TI **Hair** dyes containing benzoxadiazole, benzothiadiazole and benzo-selenadiazole derivatives
IN Pasquier, Cecile; Charriere, Veronique; Braun, Hans-Juergen
PA Wella Aktiengesellschaft, Germany
SO PCT Int. Appl., 44 pp.
CODEN: PIXXD2
DT Patent
LA German
IC ICM A61K007-13
CC 62-3 (Essential Oils and Cosmetics)
Section cross-reference(s): 41
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2002022093	A1	20020321	WO 2001-EP7494	20010629
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
	DE 10045600	A1	20020404	DE 2000-10045600	20000915
	AU 2001081924	A5	20020326	AU 2001-81924	20010629
	BR 2001007215	A	20020709	BR 2001-7215	20010629
	EP 1328244	A1	20030723	EP 2001-960429	20010629
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
	US 2003070239	A1	20030417	US 2002-110116	20020405
PRAI	DE 2000-10045600	A	20000915		
	WO 2001-EP7494	W	20010629		

GI



I

AB The invention relates to an agent for coloring fibers (A) which is produced by mixing two components (A1) and (A2) and is characterized in that the component (A1) contains at least one compd. of formula (I), wherein X represents a halogen atom, a methoxy group or an ethoxy group; Y represents an oxygen atom, a sulfuric atom or a selenium atom; and R1 and R2 can be identical or different and represent independently from each other hydrogen, a halogen atom, an (C1-C4) alkyl group, an (C1-C4) alkyl group substituted by a halogen atom, an (C1-C4) alkoxy group, a nitro group, an acetamido group or a NRaRb group, whereby the radicals Ra and Rb can be identical or different and represent independently from each other hydrogen, an (C1-C4) alkyl group, an optionally substituted carbocycle or an (C1-C4) alkane carbonyl group, or Ra and Rb form, together with the nitrogen atom, a heterocyclic (C3-C6) group; and the component (A2) contains at least one compd. from the group comprising amines, aminonitrobenzenes and phenoles. The invention also relates to a method for coloring **hair** by using the agent and a multiple component kit. Thus a **hair** dye was prepd. Component A1 contained (g): 7-chloro-4-nitro-2,1,3-benzoxadiazole 0.5; ethanol 5.0; decylpolyglycoside aq. soln. (Plantaren 2000) 4.0; EDTA sodium salt hydrate 0.2; water to 100. Components A2 was 0.153 g ethanol amine.

ST **hair** dye benzoxadiazole benzothiadiazole benzoselenadiazole deriv amine phenol

IT **Hair** preparations
(dyes; **hair** dyes contg. benzoxadiazole, benzothiadiazole and benzo-selenadiazole derivs.)

IT 95-55-6, 2-Aminophenol 99-98-9, 4-Dimethylaminoaniline 106-44-5, 4-Methylphenol, biological studies 106-50-3, 1,4-Diaminobenzene, biological studies 108-45-2, 1,3-Diaminobenzene, biological studies 108-46-3, 1,3-Dihydroxybenzene, biological studies 108-95-2, Phenol, biological studies 123-30-8, 4-Aminophenol 123-31-9, Hydroquinone, biological studies 141-43-5, Ethanol amine, biological studies 525-64-4, 2,7-Diamino fluorene 591-27-5, 3-Aminophenol 1198-27-2, 2-Naphthalenol, 1-amino-,hydrochloride 1953-54-4, 5-Hydroxyindole 2207-29-6 2274-63-7 2835-95-2, 5-Amino-2-methylphenol 2835-99-6, 4-Amino-3-methylphenol 3240-72-0, 5,6-Diamino-2,4-dihydroxypyrimidine 3523-28-2 4338-98-1 6358-09-4, 2-Amino-6-chloro-4-nitrophenol 6369-59-1, 1,4-Benzenediamine, 2-methyl-, sulfate 10199-89-0, 7-Chloro-4-nitro-2,1,3-benzoxadiazole 15639-38-0 15639-43-7 15944-78-2 16322-19-3 16461-98-6, 1H-Pyrazole-3,4-diamine **18333-73-8** 18392-74-0 18392-77-3 18392-78-4, 4-Bromo-5-methyl-7-nitro-2,1,3-benzothiadiazole 18453-42-4 19951-28-1 19951-33-8 20718-28-9 20718-47-2 20718-48-3 23920-15-2 26455-21-0 26460-78-6 29270-56-2, 4-Fluoro-7-nitro-2,1,3-benzoxadiazole 29705-39-3 32014-70-3 33229-34-4 35128-56-4 45514-38-3, 4,5-Diamino-1-methyl-1H-pyrazole 49647-58-7,

2,4,5,6-Tetraaminopyrimidine sulfate 52120-98-6 56932-44-6
62625-14-3 65235-31-6, 4-[(2-Hydroxyethyl)amino]-3-nitrophenol
66170-46-5, 1,4-Benzenediamine, 2-methyl-, hydrochloride 68579-76-0
69825-83-8 70643-19-5, 2,4-Diamino-1-(2-hydroxyethoxy)benzene
70733-34-5 71005-35-1 **81432-10-2** 81892-72-0,
1,3-Di(2,4-diaminophenoxy)propane 83763-47-7, 2-Amino-4-[(2-
hydroxyethyl)amino]anisole 89365-28-6 89365-31-1 89365-32-2
89793-88-4 90841-38-6 91267-92-4 93841-24-8, 1,4-Diamino-2-(2-
hydroxyethyl)benzene 93841-25-9 94158-13-1 95576-89-9 100418-33-5,
4-[(2-Hydroxyethyl)amino]-3-nitro-1-methylbenzene 104516-93-0
125292-42-4 131202-67-0 131202-71-6 131311-66-5 131657-78-8,
2-Chloro-6-ethylamino-4-nitrophenol 132885-85-9 155601-16-4
155601-17-5, 4,5-Diamino-1-(2-hydroxyethyl)-1H-pyrazole 157469-54-0
164919-03-3 227199-11-3 257932-06-2 257932-07-3 329320-36-7,
1,4-Diamino-2-(1-hydroxyethyl)benzene 364343-79-3 404839-62-9
404839-63-0 404839-64-1
RL: COS (Cosmetic use); BIOL (Biological study); USES (Uses)
(**hair** dyes contg. benzoxadiazole, benzothiadiazole and benzo-selenadiazole derivs.)

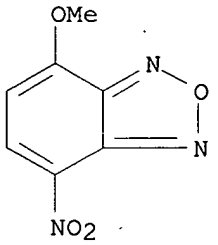
RE.CNT 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

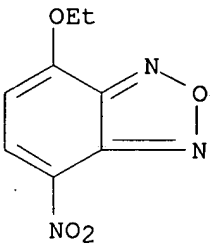
(1) Bachmann, H; US 4620850 A 1986 HCAPLUS
(2) Botta, N; US 5055110 A 1991 HCAPLUS
(3) Oberkobusch, D; WO 0110379 A 2001 HCAPLUS
(4) Oberkobusch, D; WO 0147485 A 2001
(5) Pilgram, K; US 3577427 A 1971 HCAPLUS

IT **18333-73-8 81432-10-2**
RL: COS (Cosmetic use); BIOL (Biological study); USES (Uses)
(**hair** dyes contg. benzoxadiazole, benzothiadiazole and benzo-selenadiazole derivs.)

RN 18333-73-8 HCAPLUS
CN 2,1,3-Benzoxadiazole, 4-methoxy-7-nitro- (9CI) (CA INDEX NAME)



RN 81432-10-2 HCAPLUS
CN 2,1,3-Benzoxadiazole, 4-ethoxy-7-nitro- (9CI) (CA INDEX NAME)



L32 ANSWER 5 OF 9 HCAPLUS COPYRIGHT 2003 ACS on STN
AN 2000:368704 HCAPLUS
DN 133:14300
TI In situ method of analyzing cells by staining with multiple stains and using a spectral data collection device
IN Garini, Yuval; Mcnamara, George; Soenksen, Dirk G.; Cabib, Dario; Buckwald, Robert A.
PA Applied Spectral Imaging Ltd., Israel
SO PCT Int. Appl., 129 pp.
CODEN: PIXXD2
DT Patent
LA English
IC ICM G01N033-53
ICS C12Q001-54; C12Q001-28; C12Q001-00; C12Q001-42
CC 9-4 (Biochemical Methods)
Section cross-reference(s): 3, 14
FAN.CNT 6

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2000031534	A1	20000602	WO 1999-US27000	19991116
	W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
	DE 29624210	U1	20010628	DE 1996-29624210	19961210
	US 6165734	A	20001226	US 1998-196690	19981120
	EP 1131631	A1	20010912	EP 1999-963904	19991116
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
	JP 2002530676	T2	20020917	JP 2000-584297	19991116
PRAI	US 1998-196690	A	19981120		
	US 1995-571047	A1	19951212		
	EP 1996-944834	A	19961210		
	US 1998-122704	A2	19980727		
	WO 1999-US27000	W	19991116		

AB A method of in situ anal. of a biol. sample comprises the steps of (a) staining the biol. sample with N stains of which a first stain is selected from the group consisting of a first immunohistochem. stain, a first histol. stain and a first DNA ploidy stain, and a second stain is selected from the group consisting of a second immunohistochem. stain, a second

histol. stain and a second DNA ploidy stain, with provisions that N is an integer greater than three and further that (i) if the first stain is the first immunohistochem. stain then the second stain is either the second histol. stain or the second DNA ploidy stain; (ii) if the first stain is the first histol. stain then the second stain is either the second immunohistochem. stain or the second DNA ploidy stain; whereas (iii) if the first stain is the first DNA ploidy stain then the second stain is either the second immunohistochem. stain or the second histol. stain; and (b) using a spectral data collection device for collecting spectral data from the biol. sample, the spectral data collection device and the N stains are selected so that a spectral component assocd. with each of the N stains is collectible. Figure (1) shows a block diagram illustrating the main components of an imaging spectrometer. Breast cancer tissue samples were stained with two histol. stains (hematoxylin and eosin), and four immunohistochem. stains (DAB, AEC, Fast Red, and BCIP/NBT) and measured using the Spectracube system.

ST cell analysis immunohistochem histochem DNA ploidy stain; imaging spectrometer cell analysis staining

IT Dyes
(Alexa; in situ method of analyzing cells by staining with multiple stains and using a spectral data collection device)

IT Antigens
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(CA 15-3, antibody to; in situ method of analyzing cells by staining with multiple stains and using a spectral data collection device)

IT CD antigens
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(CD100, antibody to; in situ method of analyzing cells by staining with multiple stains and using a spectral data collection device)

IT CD antigens
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(CD39, antibody to; in situ method of analyzing cells by staining with multiple stains and using a spectral data collection device)

IT CD antigens
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(CD9, antibody to; in situ method of analyzing cells by staining with multiple stains and using a spectral data collection device)

IT CD antigens
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(CD99, antibody to; in situ method of analyzing cells by staining with multiple stains and using a spectral data collection device)

IT Proteins, specific or class
RL: ARG (Analytical reagent use); BUU (Biological use, unclassified); ANST (Analytical study); BIOL (Biological study); USES (Uses)
(DNA-binding, fusion protein with green fluorescent protein, as DNA ploidy stain; in situ method of analyzing cells by staining with multiple stains and using a spectral data collection device)

IT Cadherins
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(E-, antibody to; in situ method of analyzing cells by staining with multiple stains and using a spectral data collection device)

IT Dyes

(IR, as label; in situ method of analyzing cells by staining with multiple stains and using a spectral data collection device)

IT Immunoglobulin receptors
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(IgE type II, antibody to; in situ method of analyzing cells by staining with multiple stains and using a spectral data collection device)

IT Blood-group substances
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(Lex, antibody to; in situ method of analyzing cells by staining with multiple stains and using a spectral data collection device)

IT Cell adhesion molecules
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(PECAM-1, antibody to; in situ method of analyzing cells by staining with multiple stains and using a spectral data collection device)

IT Transcription factors
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(Rb, antibody to; in situ method of analyzing cells by staining with multiple stains and using a spectral data collection device)

IT Proteins, specific or class
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(S-100, antibody to; in situ method of analyzing cells by staining with multiple stains and using a spectral data collection device)

IT Blood-group substances
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(Tn, antibody to; in situ method of analyzing cells by staining with multiple stains and using a spectral data collection device)

IT Cell adhesion molecules
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(VCAM-1, antibody to; in situ method of analyzing cells by staining with multiple stains and using a spectral data collection device)

IT Melanosome
(antibody to; in situ method of analyzing cells by staining with multiple stains and using a spectral data collection device)

IT CA 125 (carbohydrate antigen)
CA19-9 antigen
CD14 (antigen)
CD19 (antigen)
CD20 (antigen)
CD22 (antigen)
CD3 (antigen)
CD30 (antigen)
CD34 (antigen)
CD38 (antigen)
CD4 (antigen)
CD45 (antigen)
CD45RA (antigen)
CD45RO (antigen)
CD5 (antigen)
CD7 (antigen)
CD8 (antigen)

Carcinoembryonic antigen
Epidermal growth factor receptors
Estrogen receptors
Fas antigen
Fibrins
Keratins
Ki-67 antigen
P-glycoproteins
Progesterone receptors
Proliferating cell nuclear antigen
Prostate-specific antigen
Ras proteins
Transferrin receptors
Vimentins
neu (receptor)
p53 (protein)
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(antibody to; in situ method of analyzing cells by staining with multiple stains and using a spectral data collection device)

IT Integrins
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(antigens CD11c, antibody to; in situ method of analyzing cells by staining with multiple stains and using a spectral data collection device)

IT Aequorins
Biliproteins
Enzymes, biological studies
Heavy metals
Phycoerythrins
RL: ARG (Analytical reagent use); BUU (Biological use, unclassified); ANST (Analytical study); BIOL (Biological study); USES (Uses)
(as label; in situ method of analyzing cells by staining with multiple stains and using a spectral data collection device)

IT Fluorescent substances
(as labels; in situ method of analyzing cells by staining with multiple stains and using a spectral data collection device)

IT Proteins, specific or class
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(bcl-2, antibody to; in situ method of analyzing cells by staining with multiple stains and using a spectral data collection device)

IT Transcription factors
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(c-myc, antibody to; in situ method of analyzing cells by staining with multiple stains and using a spectral data collection device)

IT Uterus, neoplasm
(cervix, pap smear of; in situ method of analyzing cells by staining with multiple stains and using a spectral data collection device)

IT Avidins
RL: ARG (Analytical reagent use); BUU (Biological use, unclassified); ANST (Analytical study); BIOL (Biological study); USES (Uses)
(conjugates, in signal amplification system; in situ method of analyzing cells by staining with multiple stains and using a spectral data collection device)

IT Staining, biological

Stains, biological
(fluorescent; in situ method of analyzing cells by staining with multiple stains and using a spectral data collection device)

IT Proteins, specific or class
RL: ARG (Analytical reagent use); BUU (Biological use, unclassified); ANST (Analytical study); BIOL (Biological study); USES (Uses)
(green fluorescent, fusion protein with DNA-binding protein, as DNA ploidy stain; in situ method of analyzing cells by staining with multiple stains and using a spectral data collection device)

IT Proteins, specific or class
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(human papillomavirus, antibody to; in situ method of analyzing cells by staining with multiple stains and using a spectral data collection device)

IT Chromosome
(human, DNA probes for, labeled with fluorophores; in situ method of analyzing cells by staining with multiple stains and using a spectral data collection device)

IT Immunoassay
(immunohistochem.; in situ method of analyzing cells by staining with multiple stains and using a spectral data collection device)

IT Antibodies
RL: ARG (Analytical reagent use); BPR (Biological process); BSU (Biological study, unclassified); BUU (Biological use, unclassified); ANST (Analytical study); BIOL (Biological study); PROC (Process); USES (Uses)
(in immunohistochem. staining; in situ method of analyzing cells by staining with multiple stains and using a spectral data collection device)

IT Avidins
RL: ARG (Analytical reagent use); BUU (Biological use, unclassified); ANST (Analytical study); BIOL (Biological study); USES (Uses)
(in signal amplification system; in situ method of analyzing cells by staining with multiple stains and using a spectral data collection device)

IT Algorithm
Animal tissue
Biological materials
Cell
Colorimetry
Fluorescent dyes
Histochemistry
Imaging
Interferometry
Luminescence
Optical dispersion
Optical filters
Ploidy
Spectroscopy
Staining, biological
Stains, biological
(in situ method of analyzing cells by staining with multiple stains and using a spectral data collection device)

IT Nucleic acid hybridization
(in situ, fluorescence; in situ method of analyzing cells by staining with multiple stains and using a spectral data collection device)

IT Antibodies
RL: ARG (Analytical reagent use); BPR (Biological process); BSU

(Biological study, unclassified); BUU (Biological use, unclassified); ANST (Analytical study); BIOL (Biological study); PROC (Process); USES (Uses)
(labeled; in situ method of analyzing cells by staining with multiple stains and using a spectral data collection device)

IT Immunoglobulins
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(light chains, antibody to; in situ method of analyzing cells by staining with multiple stains and using a spectral data collection device)

IT Mammary gland
(neoplasm, tissue; in situ method of analyzing cells by staining with multiple stains and using a spectral data collection device)

IT Fusion proteins (chimeric proteins)
RL: ARG (Analytical reagent use); BUU (Biological use, unclassified); ANST (Analytical study); BIOL (Biological study); USES (Uses)
(of DNA binding protein and green fluorescent protein, as DNA ploidy stain; in situ method of analyzing cells by staining with multiple stains and using a spectral data collection device)

IT DNA
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(ploidy, stain for; in situ method of analyzing cells by staining with multiple stains and using a spectral data collection device)

IT Human papillomavirus
(proteins of, antibody to; in situ method of analyzing cells by staining with multiple stains and using a spectral data collection device)

IT Antigens
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(tau, antibody to; in situ method of analyzing cells by staining with multiple stains and using a spectral data collection device)

IT Prostate gland
Uterus
(tissue of; in situ method of analyzing cells by staining with multiple stains and using a spectral data collection device)

IT Complement receptors
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(type 1, antibody to; in situ method of analyzing cells by staining with multiple stains and using a spectral data collection device)

IT Microscopy
(with Spectracube system; in situ method of analyzing cells by staining with multiple stains and using a spectral data collection device)

IT Fluorescent substances
(with high affinity for DNA, as DNA ploidy stain; in situ method of analyzing cells by staining with multiple stains and using a spectral data collection device)

IT Integrins
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(.alpha.IIb, antibody to; in situ method of analyzing cells by staining with multiple stains and using a spectral data collection device)

IT 846-70-8, Naphthol yellow S
RL: ARG (Analytical reagent use); BUU (Biological use, unclassified); ANST (Analytical study); BIOL (Biological study); USES (Uses)
(Feulgen reaction, as histol. stain; in situ method of analyzing cells by staining with multiple stains and using a spectral data collection

device)

IT 9025-26-7, Cathepsin D 9054-63-1, CD antigens, cd13 60267-61-0, Ubiquitin 71208-06-5, Lewis X 82707-54-8, CD10 (antigen)
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(antibody to; in situ method of analyzing cells by staining with multiple stains and using a spectral data collection device)

IT 65-61-2, Acridine Orange 1239-45-8, Ethidium Bromide 7059-24-7, Chromomycin A 3
RL: ARG (Analytical reagent use); BUU (Biological use, unclassified); ANST (Analytical study); BIOL (Biological study); USES (Uses)
(as DNA ploidy stain; in situ method of analyzing cells by staining with multiple stains and using a spectral data collection device)

IT 83-89-6, Quinacrine 25535-16-4, Propidium Iodide
RL: ARG (Analytical reagent use); BUU (Biological use, unclassified); ANST (Analytical study); BIOL (Biological study); USES (Uses)
(as histol. stain, as DNA ploidy stain; in situ method of analyzing cells by staining with multiple stains and using a spectral data collection device)

IT 61-73-4, Methylene Blue 92-32-0 553-24-2, Neutral Red 633-03-4, Ethyl green 635-78-9, Resorufin 2321-07-5D, Fluorescein, reaction product with phalloidin 5141-20-8, Light Green SF 17372-87-1, Eosin 17466-45-4D, Phalloidin, reaction product with fluorescein 23491-45-4, Hoechst 33258 23491-52-3, Hoechst 33342 27072-45-3, Fluorescein isothiocyanate 47165-04-8, 4',6-Diamidino-2-phenylindole 51811-82-6, Giemsa 54327-10-5, Methyl Green 81604-88-8, Orange G
RL: ARG (Analytical reagent use); BUU (Biological use, unclassified); ANST (Analytical study); BIOL (Biological study); USES (Uses)
(as histol. stain; in situ method of analyzing cells by staining with multiple stains and using a spectral data collection device)

IT 53-57-6, NADPH 58-68-4, NADH 60-18-4, L-Tyrosine, biological studies 73-22-3, L-Tryptophan, biological studies 146-14-5, FAD 1461-15-0, Calcein 2321-07-5, Fluorescein 9001-37-0, Glucose oxidase 9001-78-9 9003-99-0, Peroxidase 9014-00-0, Luciferase 9031-11-2, .beta.-Galactosidase 13558-31-1D, derivs. 41085-99-8 53213-83-5, DiOC7(3) 69432-00-4, Calcofluor White 82354-19-6, Texas Red **88235-25-0** 98285-52-0, Spectrum Orange 102185-03-5, Cy2 138026-71-8, BODIPY 146368-14-1, Cy5 146368-16-3, Cy3 148504-34-1, Calcein-AM 159501-37-8, Cyclic GDP-Ribose 167095-09-2, MitoTracker Red 169799-14-8, Cy 7 172971-77-6 172971-78-7 189767-45-1, Cy 3.5 189767-52-0, FluorX 195395-80-3, Spectrum Green 220356-37-6, VECTOR Red 223786-97-8, Spectrum Aqua 272457-05-3, Cy 0 272457-06-4, Cy 0.5 272457-19-9, Cy 1 (dye) 272457-27-9, Cy 1.5 272457-33-7, CryptoFluor S 272457-83-7, Spectrum Blue 272457-89-3, Spectrum Gold 272458-01-2, Spectrum Red
RL: ARG (Analytical reagent use); BUU (Biological use, unclassified); ANST (Analytical study); BIOL (Biological study); USES (Uses)
(as label; in situ method of analyzing cells by staining with multiple stains and using a spectral data collection device)

IT 56-65-5, ATP, biological studies 2591-17-5, Luciferin 7440-70-2, Calcium, biological studies 55779-48-1, Coelenterazine
RL: ARG (Analytical reagent use); BUU (Biological use, unclassified); ANST (Analytical study); BIOL (Biological study); USES (Uses)
(as substrates; in situ method of analyzing cells by staining with multiple stains and using a spectral data collection device)

IT 58-85-5, Biotin
RL: ARG (Analytical reagent use); BUU (Biological use, unclassified); ANST (Analytical study); BIOL (Biological study); USES (Uses)

(in signal amplification system; in situ method of analyzing cells by staining with multiple stains and using a spectral data collection device)

IT 82446-52-4, Lucifer Yellow
RL: ARG (Analytical reagent use); BPR (Biological process); BSU (Biological study, unclassified); BUU (Biological use, unclassified); ANST (Analytical study); BIOL (Biological study); PROC (Process); USES (Uses)
(in situ method of analyzing cells by staining with multiple stains and using a spectral data collection device)

IT 58-85-5D, Biotin, antibody conjugates 298-83-9, NBT 517-28-2, Hematoxylin 1448-16-4, DAB 1672-46-4D, Digoxigenin, conjugates with DNA and rhodamine 6409-77-4, Nuclear Fast Red 7240-90-6, X-Gal 8005-77-4, Bismarck brown Y 9013-20-1D, Streptavidin, antibody conjugates 38404-93-2, BCIP 77045-20-6, Fast Red 272459-19-5, Vecor SG
RL: ARG (Analytical reagent use); BUU (Biological use, unclassified); ANST (Analytical study); BIOL (Biological study); USES (Uses)
(in situ method of analyzing cells by staining with multiple stains and using a spectral data collection device)

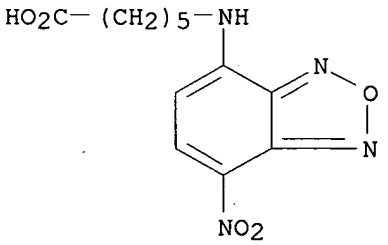
IT 2465-27-2, Auramine O 65589-70-0, Acriflavine
RL: ARG (Analytical reagent use); BUU (Biological use, unclassified); ANST (Analytical study); BIOL (Biological study); USES (Uses)
(reaction product with Feulgen, as DNA ploidy stain; in situ method of analyzing cells by staining with multiple stains and using a spectral data collection device)

IT 9013-20-1, Streptavidin
RL: ARG (Analytical reagent use); BUU (Biological use, unclassified); ANST (Analytical study); BIOL (Biological study); USES (Uses)
(with antibody; in situ method of analyzing cells by staining with multiple stains and using a spectral data collection device)

RE.CNT 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE
(1) McNamara; US 6007996 A 1999 HCAPLUS

IT **88235-25-0**
RL: ARG (Analytical reagent use); BUU (Biological use, unclassified); ANST (Analytical study); BIOL (Biological study); USES (Uses)
(as label; in situ method of analyzing cells by staining with multiple stains and using a spectral data collection device)

RN 88235-25-0 HCAPLUS
CN Hexanoic acid, 6-[(7-nitro-2,1,3-benzoxadiazol-4-yl)amino]- (9CI) (CA INDEX NAME)



L32 ANSWER 6 OF 9 HCAPLUS COPYRIGHT 2003 ACS on STN
AN 1989:53390 HCAPLUS
DN 110:53390

TI Synthesis of pyrenesulfonylamido-sphingomyelin and its use as substrate for determining sphingomyelinase activity and diagnosing Niemann-Pick disease

AU Klar, Rachel; Levade, Thierry; Gatt, Shimon
CS Hadassah Sch. Med., Hebrew Univ., Jerusalem, 91010, Israel

SO Clinica Chimica Acta (1988), 176(3), 259-67
CODEN: CCATAR; ISSN: 0009-8981
DT Journal
LA English
CC 7-1 (Enzymes)
Section cross-reference(s): 14

AB A new fluorescent deriv. of sphingomyelin (PSA 12-sphingomyelin) contg. a pyrene-sulfonylamide residue was synthesized by covalently linking 12-((1-pyrenesulfonyl)amido)-dodecanoic acid (PSA12) to sphingosylphosphorylcholine. It was used as substrate for acidic and neutral human and murine sphingomyelinases, permitting development of sensitive assays for these enzymic activities. The product of the sphingomyelinase assay, PSA12-ceramide, could be detected in picomole quantities due to a fluorescence intensity which was 10-35-fold greater than that of other fluorescent ceramides (such as pyrene or nitrobenzoxadiazole derivs.). PSA 12-sphingomyelin could be used in pure form or admixed with natural sphingomyelin; in the latter case, the enzyme hydrolyzed the fluorescent and non-fluorescent species at equal rates. Use of PSA12-sphingomyelin permitted detn. of sphingomyelinase activity in cell exts. (e.g. human blood lymphocytes, lymphoid cell lines or cultured skin fibroblasts) as well as in **hair** follicles and urine. This new fluorescent deriv. of sphingomyelin also permitted the detection of acid sphingomyelinase deficiency in cells derived from patients with Niemann-Pick disease.

ST sphingomyelinase detn sphingomyelin fluorescent deriv; Neiman Pick disease sphingomyelinase detn; pyrenesulfonylamidosphingomyelin prepn sphingomyelinase detn

IT Niemann-Pick disease
(diagnosis of, in human, detection of acid sphingomyelinase deficiency in)

IT Michaelis constant
(of sphingomyelinase, of human skin fibroblasts, with pyrenesulfonylamidododecanoyl sphingosylphosphorylcholine)

IT Fibroblast
(sphingomyelinase detn. in human, fluorescent substrate for, in Niemann-Pick disease diagnosis)

IT Lymphocyte
(sphingomyelinase detn. in, of human blood, fluorescent substrate for, in Niemann-Pick disease diagnosis)

IT Lymphoblast
(sphingomyelinase detn. in, of human skin, fluorescent substrate for, in Niemann-Pick disease diagnosis)

IT Urine analysis
(sphingomyelinase detn. in, of human, fluorescent substrate for)

IT **Hair**
(follicle, sphingomyelinase detn. in human, fluorescent substrate for)

IT Sphingomyelins
RL: SPN (Synthetic preparation); PREP (Preparation)
(N-[[(pyrenylsulfonyl)amino]lauroyl], prepn. and use in sphingomyelinase detn. and Niemann-Pick disease diagnosis)

IT 9031-54-3, Sphingomyelinase
RL: BIOL (Biological study)
(acidic and neutral, detn. of, in human and lab. animal in health and

Niemann-Pick disease, fluorescent substrate for)

IT 118540-32-2
RL: BIOL (Biological study)
(condensation of, with pyrenesulfonylamidododecanoic acid)

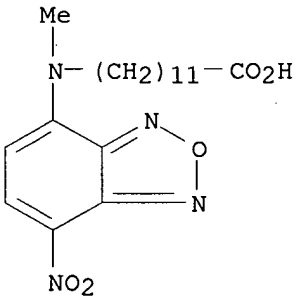
IT **73025-01-1** 111864-04-1
RL: BIOL (Biological study)
(condensation of, with sphingosylphosphorylcholine)

IT 118578-43-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and use in human and lab. animal sphingomyelinase detn. in health and Niemann-Pick disease)

IT **118540-33-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and use in sphingomyelinase detn. and Niemann-Pick disease diagnosis)

IT **73025-01-1**
RL: BIOL (Biological study)
(condensation of, with sphingosylphosphorylcholine)

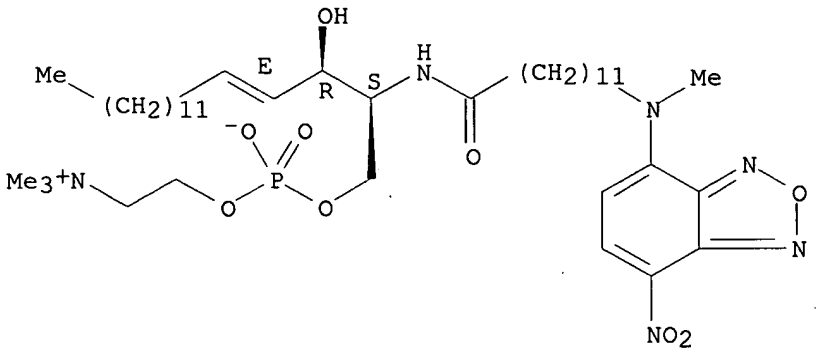
RN 73025-01-1 HCAPLUS
CN Dodecanoic acid, 12-[methyl(7-nitro-2,1,3-benzoxadiazol-4-yl)amino]- (9CI) (CA INDEX NAME)



IT **118540-33-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and use in sphingomyelinase detn. and Niemann-Pick disease diagnosis)

RN 118540-33-3 HCAPLUS
CN 18,20-Dioxa-2,15-diaza-19-phosphadocosan-22-aminium, 19-hydroxy-16-(1-hydroxy-2-pentadecenyl)-N,N,N-trimethyl-2-(7-nitro-2,1,3-benzoxadiazol-4-yl)-14-oxo-, inner salt, 19-oxide, [R-[R*,S*-(E)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



L32 ANSWER 7 OF 9 HCAPLUS COPYRIGHT 2003 ACS on STN
AN 1988:607706 HCAPLUS
DN 109:207706
TI In situ localization of actin filaments in higher plant cells using fluorescent probes
AU Parthasarathy, M. V.
CS Div. Biol. Sci., Cornell Univ., Ithaca, NY, 14853, USA
SO Plant Molecular Biology Reporter (1987), 5(1), 251-9
CODEN: PMBRD4; ISSN: 0735-9640
DT Journal
LA English
CC 9-4 (Biochemical Methods)
Section cross-reference(s): 11
AB Procedures for the in situ localization of F-actin in various plant tissues, pollen, and tissue cultured cells are described, using rhodamine-phalloidin (Rh-Ph) as the fluorescent probe. 7-Nitroben-2-oxa-1,3-diazole-phallacidin can also be used as a probe, but it tends to fade faster than Rh-Ph during observation and photog. Photomicrographs indicate that actin filaments form a three-dimensional network with fine branches extending into the crit. region of the cell. F-actin is often assocd. with the nucleus and frequently appears to terminate at or near the plasma membrane. The architecture of F-actin varies, depending on the cell shape.
ST actin filament plant cell; fluorescence microscopy actin filament plant cell
IT Tobacco
(actin filament localization in cells of, fluorescent probes in evaluation of)
IT Barley
Oat
(actin filament localization in coleoptile cells of, fluorescent probes in evaluation of)
IT Cytoskeleton
Pollen
(actin localization in, fluorescent probes in evaluation of)
IT Tomato
(actin-filament localization in stem **hair** cells of, fluorescent probes in evaluation of)
IT Actins
RL: PROC (Process)
(F-, localization of, in plant cells with fluorescent probes)
IT Microscopy

(fluorescence, in actin filament localization in plant cells)

IT Fluorescent substances
(probes, actin filament localization in plant cells evaluation by)

IT Plant tissue culture
(suspension, of carrot and tobacco, actin filament localization in cells of, fluorescent probes in evaluation of)

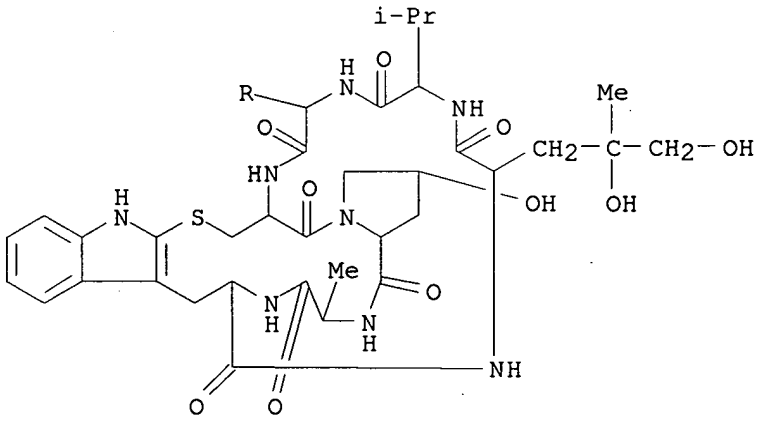
IT 509-72-8D, reaction products with phalloidin 17466-45-4D, reaction products with rhodamine **73413-78-2**
RL: ANST (Analytical study)
(actin filament localization in plant cells evaluation by)

IT **73413-78-2**
RL: ANST (Analytical study)
(actin filament localization in plant cells evaluation by)

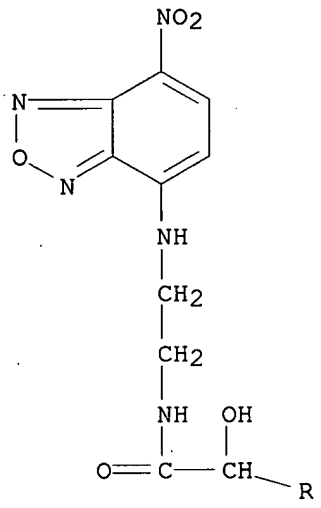
RN 73413-78-2 HCAPLUS

CN Phallacidin, 5-[erythro-3-hydroxy-N-[2-[(7-nitro-2,1,3-benzoxadiazol-4-yl)amino]ethyl]-D-asparagine]- (9CI) (CA INDEX NAME)

PAGE 1-A

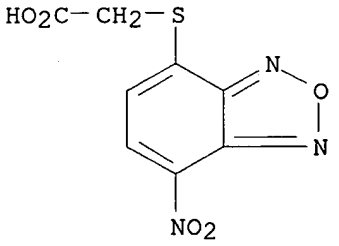


PAGE 2-A

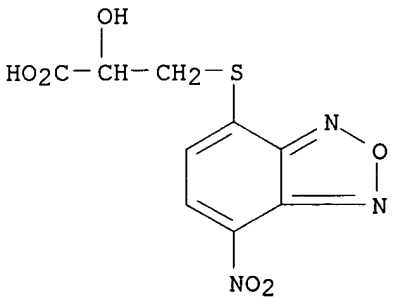


L32 ANSWER 8 OF 9 HCAPLUS COPYRIGHT 2003 ACS on STN
AN 1981:180484 HCAPLUS
DN 94:180484
TI High pressure liquid chromatography determination of thioglycolic acid in cold wave fluids and depilating creams
AU Rooselaar, J.; Liem, D. H.
CS Food Inspection Serv. Enschede, Enschede, 7500 AT, Neth.
SO International Journal of Cosmetic Science (1981), 3(1), 37-47
CODEN: IJCMDW; ISSN: 0142-5463
DT Journal
LA English
CC 62-1 (Essential Oils and Cosmetics)
AB In a high-pressure liq. chromatog. method for the detn. of thioglycolic acid [68-11-1] in **hair** waving fluids and depilatories, the acid is converted to a yellow nitrobenzoxadioazole (NBD) deriv. before chromatog. to permit detection at 464 nm. Optimum derivatization conditions could be obtained when 0.01% aq. solns. of thioglycolic acid were heated with 7-chloro-4-nitrobenz-2-oxa-1,3-diazole [10199-89-0] at pH 7. **Hair** waving fluids and depilatories are simply dild. with an aq. pH 7 buffer and, if necessary, clarified and filtered, before the derivatization procedure. An internal std., Sunset Yellow FCF, is added to the mixt. before performing ion-pair reverse-phase HPLC. A reverse phase C18 column is used. The mobile phase is aq. MeOH, to which the counter ion, tetrabutylammonium phosphate, is added. Recoveries were 97.8-100.7%. The proposed method permits a resoln. of other mercapto compds., such as thiolactic acid [79-42-5] and thioglycerol [96-27-5]. Sixty market samples of cold wave fluids and depilatories were analyzed by the proposed method, and the results were generally lower than those obtained by iodometric titrn.
ST thioglycolate detn depilatory **hair** waving; high pressure liq chromatog thioglycolate; nitrobenzoxadiazolethioglycolate chromatog
IT Depilatories
(thioglycolic acid detn. in, by high-pressure liq. chromatog.)
IT Chromatography, column and liquid
(high-pressure, of nitrobenzoxadiazole mercapto derivs.)

IT **Hair** preparations
(wave-setting, thioglycolic acid detn. in, by high-pressure liq. chromatog.)
IT 79-42-5 96-27-5 107-96-0
RL: ANT (Analyte); ANST (Analytical study)
(detn. of, by high-pressure liq. chromatog.)
IT 68-11-1, analysis
RL: ANT (Analyte); ANST (Analytical study)
(detn. of, in depilatories and **hair**-waving solns. by high-pressure liq. chromatog.)
IT **18333-81-8P 77460-15-2P 77460-16-3P 77460-17-4P**
RL: PREP (Preparation)
(prepn. of, for high-pressure liq. chromatog.)
IT 10199-89-0
RL: BIOL (Biological study)
(reaction with mercapto compds., for high-pressure liq. chromatog. anal.)
IT **18333-81-8P 77460-15-2P 77460-16-3P 77460-17-4P**
RL: PREP (Preparation)
(prepn. of, for high-pressure liq. chromatog.)
RN 18333-81-8 HCAPLUS
CN Acetic acid, [(7-nitro-2,1,3-benzoxadiazol-4-yl)thio]- (9CI) (CA INDEX NAME)

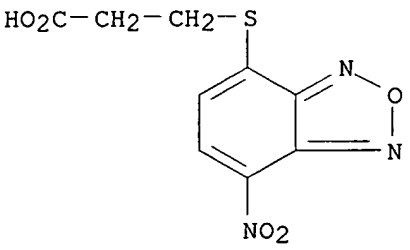


RN 77460-15-2 HCAPLUS
CN Propanoic acid, 2-hydroxy-3-[(7-nitro-2,1,3-benzoxadiazol-4-yl)thio]- (9CI) (CA INDEX NAME)

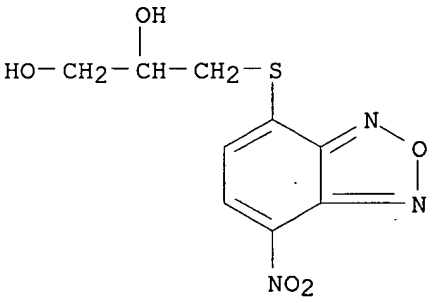


RN 77460-16-3 HCAPLUS
CN Propanoic acid, 3-[(7-nitro-2,1,3-benzoxadiazol-4-yl)thio]- (9CI) (CA

INDEX NAME)



RN 77460-17-4 HCAPLUS
CN 1,2-Propanediol, 3-[(7-nitro-2,1,3-benzoxadiazol-4-yl)thio]- (9CI) (CA INDEX NAME)



L32 ANSWER 9 OF 9 HCAPLUS COPYRIGHT 2003 ACS on STN
AN 1980:123835 HCAPLUS
DN 92:123835
TI A fluorometric determination of sphingomyelinase by use of fluorescent derivatives of sphingomyelin, and its application to diagnosis of Niemann-Pick disease
AU Gatt, S.; Dinur, T.; Barenholz, Y.
CS Hadassah Med. Sch., Hebrew Univ., Jerusalem, Israel
SO Clinical Chemistry (Washington, DC, United States) (1980), 26(1), 93-6
CODEN: CLCHAU; ISSN: 0009-9147
DT Journal
LA English
CC 7-1 (Enzymes)
Section cross-reference(s): 14
AB Fluorescent derivs. of sphingomyelin (N-acylsphingosylphosphocholine) were synthesized and used as substrates for several sphingomyelinase (I) prepns. The following 5 fluorescent probes, each attached to the terminal C atom of the fatty acyl residue, were introduced into sphingomyelin: dansyl, pyrene, carbazole, 4-chloro-7-nitrobenz-2-oxa-1,3-diazole, and anthroic acid. The rates at which the fluoro- and radiolabeled sphingomyelins were hydrolyzed were detd. The rates were the same with these 3 I prepns.: (a) a purified I from Staphylococcus aureus; (b) a Triton X-100-treated ext. of human brain (assayed at pH 7.4 in the presence of Mg2+); and (c) aq. exts. of brain lysosomes, skin fibroblasts, and amniotic cells, assayed at pH 5.0. Homogenates of skin fibroblasts of

a patient with Niemann-Pick disease had practically no activity when assayed at pH 5 with fluorosphingomyelin as substrate. When fluorosphingomyelin was mixed in various proportions with natural sphingomyelin, I from each of the 3 sources hydrolyzed the 2 substrates at equal rates. The fluorosphingomyelins can be used to est. I activity with great sensitivity in exts. of tissues or cells, in tears, and probably in **hair** follicles, as well as diagnose Niemann-Pick disease, either pre- or postnatally.

ST sphingomyelinase detn fluorometry; Niemann Pick disease diagnosis sphingomyelinase; sphingomyelin fluorescent deriv prepn

IT Niemann-Pick disease
(diagnosis of, sphingomyelinase detn. in)

IT Amniotic fluid
(sphingomyelinase detn. in cells of, prenatal Nieman-Pick Disease diagnosis in relation to)

IT Fibroblast
(sphingomyelinase detn. in, Niemann-Pick Disease diagnosis in relation to)

IT Sphingomyelins
(fluorescent fatty acid-contg., prepn. and use in sphingomyelinase detn.)

IT 60177-21-1 64821-29-0 69168-45-2 73024-99-4 73025-00-0
73025-01-1 73025-02-2 73038-57-0
RL: BIOL (Biological study)
(condensation of, with sphingosylphosphocholine)

IT 9031-54-3
RL: ANT (Analyte); ANST (Analytical study)
(detn. of, fluorometric, in Niemann-Pick Disease diagnosis)

IT **73025-01-1**
RL: BIOL (Biological study)
(condensation of, with sphingosylphosphocholine)

RN 73025-01-1 HCAPLUS

CN Dodecanoic acid, 12-[methyl(7-nitro-2,1,3-benzoxadiazol-4-yl)amino]- (9CI) (CA INDEX NAME)